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Sommario/riassunto

This book offers a unique “learn-by-tutorial” approach for ab initio quantum Monte Carlo (QMC) electronic state calculations. The ab initio QMC method is a representative “Beyond DFT” technique that overcomes challenges faced by the widely used density functional theory (DFT) in materials science. This is the first book focusing on simulation operations of ab initio QMC methods in a tutorial format. This book explains the theoretical background of the ab initio QMC method as a showcase of many-body electron theory attracting interest also from fundamental scientists dealing with quantum many-body problems. The content of this book is written in an accessible manner, targeting the same audience as the author’s previous work, “Ab initio Calculation Tutorial: For Materials Analysis, Informatics and Design.” It is structured to allow beginners in simulation from experimental fields and industry to set up practice codes on their personal PCs and learn independently, without assuming prior knowledge of many-body electron theory or simulation science. Readers learn how to solve the problems on intermolecular binding forces in biomolecular systems, magnetic descriptions in spintronics, and material properties involving discontinuous density distributions such as surfaces, interfaces, and defects.